

# ANALYSIS OF SCHRÖDINGER OPERATORS WITH INVERSE SQUARE POTENTIALS II: FEM AND APPROXIMATION OF EIGENFUNCTIONS IN THE PERIODIC CASE

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ABSTRACT. Let  $V$  be a *periodic* potential on  $\mathbb{R}^3$  that is smooth everywhere except at a discrete set  $\mathcal{S}$  of points, where it has singularities of the form  $Z/\rho^2$ , with  $\rho(x) = |x - p|$  for  $x$  close to  $p$  and  $Z$  is continuous,  $Z(p) > -1/4$  for  $p \in \mathcal{S}$ . We also assume that  $\rho$  and  $Z$  are smooth outside  $\mathcal{S}$  and  $Z$  is smooth in polar coordinates around each singular point. Let us denote by  $\Lambda$  the periodicity lattice and set  $\mathbb{T} := \mathbb{R}^3/\Lambda$ . In the first paper of this series [20], we obtained regularity results in weighted Sobolev space for the eigenfunctions of the Schrödinger-type operator  $H = -\Delta + V$  acting on  $L^2(\mathbb{T})$ , as well as for the induced  $\mathbf{k}$ -Hamiltonians  $H_{\mathbf{k}}$  obtained by restricting the action of  $H$  to Bloch waves. In this paper we present two related applications: one to the Finite Element approximation of the solution of  $(L + H_{\mathbf{k}})v = f$  and one to the numerical approximation of the eigenvalues,  $\lambda$ , and eigenfunctions,  $u$ , of  $H_{\mathbf{k}}$ . We give optimal, higher order convergence results for approximation spaces defined piecewise polynomials. Our numerical tests are in good agreement with the theoretical results.

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## 1. INTRODUCTION AND STATEMENT OF MAIN RESULTS

In this paper, which is the second part of work begun in [20], we present applications of the theoretical regularity results in the first part of this paper to Finite Element Method approximation schemes. The first application is to approximation of eigenvalues,  $\lambda$ , and eigenfunctions,  $u$ , of the Bloch operator,  $H_{\mathbf{k}}$ , associated to a periodic Hamiltonian operator with inverse square potential at isolated points. For example, one of our main results, Theorem 1.1 yields optimal orders of convergence for the Finite Element approximations of the eigenvalues of  $H_{\mathbf{k}}$  using graded meshes. These rates are higher than those that can be obtained using standard meshes. The second application is to the Finite Element Method, again using graded meshes, applied to equations of

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the form  $(L + H_{\mathbf{k}})v = f$ . The final section of this paper presents numerical tests showing good agreement with our theoretical results for this second problem.

Hamiltonian operators with inverse square potentials arise in a variety of interesting contexts. The standard example of a Schrödinger operator with  $c/\rho$  potential is a special case of the inverse square potentials we consider, where the function  $\rho^2 V$  vanishes to order 1 at the singularity, and the results of this work apply to such operators. But in addition, Hamiltonians with true inverse square potentials arise in relativistic quantum mechanics from the square of the Dirac operator coupled with an interaction potential, and they arise in the interaction of a polar molecule with an electron. See [29, 32] for further applications of inverse square potentials to physics. See also [1, 19, 25, 28, 9] for related results on operators with singular coefficients. Thus it is interesting in several areas of physics to understand how to approximate solutions to equations involving such operators.

Before we can state our approximation results, we must fix some notation and state the assumptions we make about our Hamiltonian operators. Consider a Hamiltonian operator  $H := -\Delta + V$  that is periodic on  $\mathbb{R}^3$  with triclinic periodicity lattice  $\Lambda$ . Its fundamental domain is a parallelepiped whose faces can be identified under the symmetries of  $H$  to form the torus  $\mathbb{T} = \mathbb{R}^3/\Lambda$ , which is how we will denote this fundamental domain in the remainder of this paper. Let  $\rho(x)$  be a continuous function on  $\mathbb{T}$  that is given by  $\rho(x) = |x - p|$  for  $x$  close to  $p$ , is smooth except at the points of  $\mathcal{S}$ , and may be assumed to be equal to one outside a neighbourhood of  $\mathcal{S}$ .

We need two assumptions about the potentials  $V$  that we will consider in this paper. First, we assume that  $V$  is smooth except at a set of points  $\mathcal{S} \subset \mathbb{T}$ , near which it has singularities of the form  $Z/\rho^2$ , where  $Z$  is continuous on  $\mathbb{T}$  and smooth in polar coordinates around  $p$ . We denote this as follows.

$$(1) \quad \textbf{Assumption 1 :} \quad Z := \rho^2 V \in \mathcal{C}(\mathbb{T}) \cap \mathcal{C}^\infty(\overline{\mathbb{T} \setminus \mathcal{S}}).$$

Assumption 1, more precisely the continuity of  $Z$  at  $\mathcal{S}$ , allows us to formulate our second assumption. Namely,

$$(2) \quad \textbf{Assumption 2 :} \quad \eta := \min_{p \in \mathcal{S}} \sqrt{1/4 + Z(p)} > 0.$$

In particular, we assume that for all  $p \in \mathcal{S}$ ,  $Z(p) > -1/4$ . These assumptions are sharp in the sense that the analysis yields fundamentally different results if either one fails. In particular, the value  $\eta = -1/4$  corresponds to the critical coupling for an isolated inverse square potential in  $\mathbb{R}^3$  where the system undergoes a transition between the conformal and non-conformal regimes [29]. If the first assumption fails, then the available analytic techniques are much weaker, see for instance [17, 16]. In either case, the approximation theorems in this paper fail if either assumption is violated. More details of this are included in the first part, [20], and a study of the analysis when these assumptions are relaxed will be examined in a forthcoming paper.

We are interested in understanding the spectrum and generalised eigenfunctions of the operator  $H$ . As usual, we do this by studying Bloch waves. Recall that if  $\mathbf{k}$  is an element of the first Brillion zone of  $\Lambda$ , that is, is an element of the fundamental domain of the dual lattice of  $\Lambda$ , then a Bloch wave with wave vector  $\mathbf{k}$  is a function in  $L^2_{loc}(\mathbb{R}^3)$  that satisfies the semi-periodicity condition

$$(3) \quad \psi_{\mathbf{k}}(x + X) = e^{i\mathbf{k} \cdot X} \psi_{\mathbf{k}}(x) \quad \forall X \in \Lambda.$$

It is well known that such a Bloch wave can be written as

$$(4) \quad \psi_{\mathbf{k}}(x) = e^{i\mathbf{k} \cdot x} u_{\mathbf{k}}(x)$$

for a function  $u_{\mathbf{k}}$  that is truly periodic with respect to  $\Lambda$  and thus can be considered as living on the three-torus  $\mathbb{T}$ . We define the  $\mathbf{k}$ -Hamiltonian  $H_{\mathbf{k}}$  on  $L^2(\mathbb{T})$  by

$$(5) \quad H_{\mathbf{k}} := - \sum_{j=1}^3 (\partial_j + i k_j)^2 + V.$$

Then we have further that if a Bloch wave  $\psi_{\mathbf{k}}$  is a generalized eigenfunction of  $H$  with generalized eigenvalue  $\lambda$ , then the function  $u_{\mathbf{k}} := e^{-i\mathbf{k} \cdot x} \psi_{\mathbf{k}}(x)$  is a standard  $L^2$ -eigenfunction of  $H_{\mathbf{k}}$  with eigenvalue  $\lambda$ . Let  $\lambda_j$ ,  $j \geq 1$ , be the eigenvalues of  $H_{\mathbf{k}}$ , arranged in increasing order,  $\dots \leq \lambda_j \leq \lambda_{j+1} \leq \dots$ , and repeated according to their multiplicities. That is, if  $E(\lambda)$  denotes the eigenspace of  $H_{\mathbf{k}}$  corresponding to  $\lambda$ , then  $\lambda$  is repeated  $\dim(E(\lambda))$  times.

As usual, for our finite element approximation results, we consider a sequence  $S_n$  of finite dimensional subspaces of the domain of  $H_{\mathbf{k}}$  and let  $R_n$  denote the Riesz projection onto  $S_n$ , that is, the projection in the bilinear form  $((L + H_{\mathbf{k}})y, w)_{L^2(\mathbb{T} \setminus \mathcal{S})}$ , (for a suitable  $C \geq 0$ ), associated to  $H_{\mathbf{k}}$ . Let  $H_{\mathbf{k},n} := R_n H_{\mathbf{k}} R_n$  be the associated finite element approximation of  $H_{\mathbf{k}}$ , acting on  $S_n$ . Denote by  $\lambda_{j,n}$  the eigenvalues of the approximation  $H_{\mathbf{k},n}$ , again arranged in increasing order,  $\dots \leq \lambda_{j,n} \leq \lambda_{j+1,n} \leq \dots$ , and repeated according to their multiplicities and let  $u_{j,n} \in S_n$  be a choice of corresponding eigenfunctions (linearly independent). The spaces  $S_n$  we use for our theorems are defined in terms of a sequence of graded tetrahedral meshes  $\mathcal{T}_n := k^n(\mathcal{T}_0)$  on  $\mathbb{T}$  (sometimes called triangulations), given by sequential refinements, associated to a scaling parameter  $k$ , of an original tetrahedral mesh  $\mathcal{T}_0$ . We describe the meshing refinement procedure in detail in Section 3. We will take  $S_n = S(\mathcal{T}_n, m)$ , the finite element spaces associated to these meshes (*i.e.*, using continuous, piecewise polynomials of degree  $m$ ).

Our first theorem, which is a theoretical result for the finite element method approximation of eigenvalues and eigenfunctions of  $H_{\mathbf{k}}$  using tetrahedralisations with graded meshes, is as follows.

**Theorem 1.1.** *Let  $\lambda_j$  be an eigenvalue of  $H_{\mathbf{k}}$  and fix  $0 < a < \eta$ ,  $a \leq m$ . Let  $\lambda_{j,n}$  be the finite element approximations of  $\lambda_j$  associated to the nested sequence  $\mathcal{T}_n$  of meshes on  $\mathbb{T}$  defined by the scaling parameter  $k = 2^{-m/a}$  and piecewise polynomials of degree  $m$ . Also, let  $u_{j,n}$  be an eigenbasis corresponding to  $\lambda_{j,n}$ . Then there exists a constant  $c(\lambda_j, a)$  independent of  $n$  such that the following inequalities hold for a suitable eigenvector  $u_j \in E(\lambda_j)$ :*

$$|\lambda_j - \lambda_{j,n}| \leq c(\lambda_j, a) \dim(S_n)^{-2m/3},$$

$$\|u_j - u_{j,n}\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq c(\lambda_j, a) \dim(S_n)^{-m/3},$$

where the space  $\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})$  is a weighted Sobolev space defined below in Equation 9.

For our second theorem, we consider the finite element approximations of the equation

$$(6) \quad (L + H_{\mathbf{k}})v = f, \quad \text{for } L > C_0,$$

where  $C_0$  is the constant from Theorem 2.1 below. We then define the form  $a(y, w) := ((L + H_{\mathbf{k}})y, w)$  and let  $v$  be the solution of Equation (6) above. We then define the usual Galerkin Finite Element approximation  $v_n$  of  $v$  as the unique  $v_n \in S_n := S(\mathcal{T}_n, m)$  such that

$$(7) \quad a(v_n, w_n) := ((L + H_{\mathbf{k}})v_n, w_n) = (f, w), \quad \text{for all } w_n \in S_n.$$

Then Theorem 1.1 together with the Lax-Milgram Lemma and Cea's lemma imply that we have the following  $h^m$  quasi-optimal rate of convergence.

**Theorem 1.2.** *The sequence  $\mathcal{T}_n := k^n(\mathcal{T}_0)$  of meshes on  $\mathbb{P}$  defined using the  $k$ -refinement, for  $k = 2^{-m/a}$ ,  $0 < a < \eta$ ,  $a \leq m$ , and piecewise polynomials of degree  $m$ , has the following property. The sequence  $v_n \in S_n := S(\mathcal{T}_n, m)$  of Finite Element (Galerkin) approximations of  $v$  from Equation (7) satisfies*

$$(8) \quad \|v - v_n\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|f\|_{\mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})},$$

where  $C$  is independent of  $n$  and  $f$ .

These theorems are interesting because it is known that the convergence rate of a standard finite element method (*i.e.*, based on quasi-uniform meshes) is limited. However, under the assumptions on our potentials, if we use graded meshes instead, we can obtain an approximation rate as fast as we like by using polynomials of sufficiently high degree in the elements. This is due to the fact that although regularity of the associated Bloch waves is limited in terms of standard

Sobolev spaces on  $\mathbb{T}$ , it is arbitrarily good with respect to weighted Sobolev spaces. We will recall the definition of these spaces and the relevant regularity results from [20] along with additional background in Section 2.

The remainder of the paper is organised as follows. In Section 3, we first describe the  $k$ -refinement algorithm for the three dimensional tetrahedral meshes, which results in a sequence of meshes  $\mathcal{T}_n$ . We then prove a general interpolation approximation result for the sequence of finite element spaces associated to this sequence of meshes. In Section 4 we use this general approximation result to prove our main approximation results. This section includes in particular the proofs of Theorem 1.1 and Theorem 1.2, as well as an additional result about the condition number of the stiffness matrix associated to the finite element spaces,  $S_n$ . In the last section, Section 5, we discuss results of numerical tests of the method for solving equations of the form  $(L + H_{\mathbf{k}})v = f$  and compare them to the theoretical results.

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## 2. BACKGROUND RESULTS

In this section we recall some definitions and results from [20], as well as the classical approximation result for Lagrange interpolants (see [2, 11, 15, 31]), that will be used in the proofs of the approximation theorems above. First, these results are given in terms of weighted Sobolev spaces which are defined as follows:

$$(9) \quad \mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S}) := \{v : \mathbb{T} \setminus \mathcal{S} \rightarrow \mathbb{C}, \rho^{|\beta|-a} \partial^\beta v \in L^2(\mathbb{T}), \forall |\beta| \leq m\}.$$

These spaces have been considered in many other papers, most notably in Kondratiev's ground-breaking paper [24].

The first result that we recall guarantees the existence of solutions of equations of the form  $(L + H_{\mathbf{k}})v = f$  for  $L$  greater than some constant  $C_0$ , and identifies the natural domain of  $H_{\mathbf{k}}$ . Let us fix smooth functions  $\chi_p$  supported near points of  $\mathcal{S}$  such that the functions  $\chi_p$  have disjoint supports and  $\chi_p = 1$  in a small neighbourhood of  $p \in \mathcal{S}$ . Then Theorem 1.1 and Proposition 3.6 from [20] combine to give right away the following result.

**Theorem 2.1.** *Let  $V$  be a potential satisfying both Assumptions 1 and 2. Then there exists  $C_0 > 0$  such that  $L + H_{\mathbf{k}} : \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}) \rightarrow \mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})$  is an isomorphism for all  $m \in \mathbb{Z}_{\geq 0}$ , all  $|a| < \eta$ , and all  $L > C_0$ . Moreover, for any  $u \in \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S})$  satisfying  $(L + H_{\mathbf{k}})v = f \in H^{m-1}(\mathbb{T} \setminus \mathcal{S})$ , we can find constants  $a_p \in \mathbb{R}$  such that*

$$u_{reg} := u - \sum_{p \in \mathcal{S}} \chi_p \rho^{\sqrt{1/4 + Z(p)} - 1/2} \in \mathcal{K}_2^{m+1}(\mathbb{T} \setminus \mathcal{S}).$$

We obtain, in particular, that  $H_{\mathbf{k}}$  has a natural self-adjoint extension, the Friedrichs extension. Therefore, from now on, we shall extend  $H_{\mathbf{k}}$  to the domain of the Friedrichs extension of  $L + H_{\mathbf{k}}$ , as in the above Theorem. Let us denote by  $\mathcal{D}(H_{\mathbf{k}})$  its domain. Then Theorem 2.1 gives that  $\mathcal{D}(H_{\mathbf{k}}) = \mathcal{K}_2^2(\mathbb{T} \setminus \mathcal{S})$  for  $\min_p Z(p) > 3/4$ , and, in general,

$$(10) \quad \mathcal{D}(H_{\mathbf{k}}) \subset \mathcal{K}_{a+1}^2(\mathbb{T} \setminus \mathcal{S}), \quad \text{for } a < \eta := \min_p \sqrt{1/4 + Z(p)} \text{ and } a \leq 1$$

so that  $\mathcal{D}(H_{\mathbf{k}}) \subset \mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S}) \subset H^1(\mathbb{T} \setminus \mathcal{S})$ , since we assumed that  $\min_p Z(p) > -1/4$ .

We can now state a regularity theorem for the eigenfunctions of  $H_{\mathbf{k}}$  near a point  $p \in \mathcal{S}$ , or equivalently, for Bloch waves associated to the wavevector  $\mathbf{k}$ .

**Theorem 2.2.** *Assume that  $V$  satisfies Assumptions 1 and 2 and let  $u \in \mathcal{D}(H_{\mathbf{k}})$  satisfy  $H_{\mathbf{k}}u = \lambda u$ , for some  $\lambda \in \mathbb{R}$ . Then we can find constants  $a_p \in \mathbb{R}$  such that*

$$u - \sum_{p \in \mathcal{S}} \chi_p \rho^{\sqrt{1/4 + Z(p)} - 1/2} \in \mathcal{K}_{a'+1}^{m+1}(\mathbb{T} \setminus \mathcal{S}), \quad \forall a' < \min_{p \in \mathcal{S}} \sqrt{9/4 + Z(p)}.$$

*In particular,  $u \in \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S})$ , where  $a < \eta := \min_{p \in \mathcal{S}} \sqrt{1/4 + Z(p)}$  and  $m \in \mathbb{Z}_+$  is arbitrary.*

See also [22, 23] for some related classical results in this area. Theorems 2.1 and 2.2 lead to an estimate for the distance from an element in the domain of  $H_{\mathbf{k}}$  to the approximation spaces that we construct using graded meshes.

Next, recall the definition of Lagrange interpolants associated to a mesh. Let us choose  $\mathbb{P}$  to be a parallelepiped that is a fundamental domain of the Lattice  $\Lambda$ . That is,  $\mathbb{R}^3 = \cup_{y \in \Lambda} (y + \mathbb{P})$  and all  $y + \mathbb{P}$  disjoint. Let  $\mathcal{T} = \{T_i\}$  be a *mesh* on  $\mathbb{P}$ , that is a mesh of  $\mathbb{P}$  with tetrahedra  $T_i$ . We can identify this  $\mathcal{T}$  with a mesh  $\mathcal{T}'$  of the fundamental region of the lattice  $\mathcal{L}$  (that is, to the Brillouin zone of  $\mathcal{L}$ ). Fix an integer  $m \in \mathbb{N}$  that will play the role of the order of approximation. We denote by  $S(\mathcal{T}, m)$  the finite element space associated to the degree  $m$  Lagrange tetrahedron. That is,  $S(\mathcal{T}, m)$  consists of all continuous functions  $\chi : \mathbb{P} \rightarrow \mathbb{R}$  such that  $\chi$  coincides with a polynomial of degree  $\leq m$  on each tetrahedron  $T \in \mathcal{T}$  and  $\chi$  is *periodic*. This means the values of  $\chi$  on corresponding faces coincide, so  $\chi$  will have a continuous, periodic extension to the whole space, or alternatively, can be thought of as a continuous function on  $\mathcal{T}$ . We shall denote by  $w_I = w_{I,\mathcal{T}} \in S(\mathcal{T}, m)$  the Lagrange interpolant of  $w \in H^2(\mathbb{R}^3)$ . Let us recall the definition of  $w_{I,\mathcal{T}}$ . First, given a tetrahedron  $T$ , let  $[t_0, t_1, t_2, t_3]$  be the barycentric coordinates on  $T$ . The nodes of the degree  $m$  Lagrange tetrahedron  $T$  are the points of  $T$  whose barycentric coordinates  $[t_0, t_1, t_2, t_3]$  satisfy  $mt_j \in \mathbb{Z}$ . The *degree  $m$  Lagrange interpolant*  $w_{I,\mathcal{T}}$  of  $u$  is the unique function  $w_{I,\mathcal{T}} \in S(\mathcal{T}, m)$  such that  $w = w_{I,\mathcal{T}}$  at the nodes of each tetrahedron  $T \in \mathcal{T}$ . The shorter notation  $w_I$  will be used when only one mesh is understood in the discussion.

The classical approximation result for Lagrange interpolants ([2, 11, 15, 31]) can now be stated.

**Theorem 2.3.** *Let  $\mathcal{T}$  be a mesh of a polyhedral domain  $\mathbb{P} \subset \mathbb{R}^3$  with the property that all tetrahedra comprising  $\mathcal{T}$  have angles  $\geq \alpha$  and edges  $\leq h$ . Then there exists a constant  $C(\alpha, m) > 0$  such that, for any  $u \in H^{m+1}(\mathbb{P})$ ,*

$$\|u - u_I\|_{H^1(\mathbb{P})} \leq C(\alpha, m) h^m \|u\|_{H^{m+1}(\mathbb{P})}.$$

Finally, we recall two properties of functions in the weighted Sobolev spaces  $\mathcal{K}_a^m(\mathbb{T} \setminus \mathcal{S})$  that are useful for the analysis of the approximation scheme we use with graded meshes. The proofs of these lemmas are contained in [21] and are based on the definitions and straightforward calculations.

**Lemma 2.4.** *Let  $D$  be a small neighborhood of a point  $p \in \mathcal{S}$  such that on  $D$ ,  $\rho$  is given by distance to  $p$ . Let  $0 < \gamma < 1$  and denote by  $\gamma D$  the region obtained by radially shrinking around  $p$  by a factor of  $\gamma$ . Then*

$$\|w\|_{\mathcal{K}_a^m(D)} = (\gamma)^{a-3/2} \|w\|_{\mathcal{K}_a^m(\gamma D)}.$$

**Lemma 2.5.** *If  $m \geq m'$ ,  $a \geq a'$  and  $0 < \rho < \delta$  on  $D$ , then*

$$\|w\|_{\mathcal{K}_{a'}^{m'}(D)} \leq \delta^{a-a'} \|w\|_{\mathcal{K}_a^m(D)}.$$

We can now continue to the definition of the mesh refinement technique and the proof of the general approximation theorem underlying our two main theorems.

### 3. APPROXIMATION AND MESH REFINEMENT

Our two main theorems follow from standard results, such as Cea's Lemma (for the proof of Theorem 1.2) and the results used in [3, 5, 4, 10, 30] (for the proof of Theorem 1.1), together with the following underlying approximation theorem:

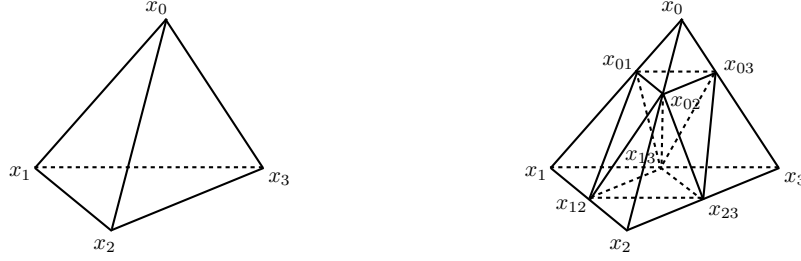


FIGURE 1. The initial tetrahedron  $\{x_0, x_1, x_2, x_3\}$  (left); eight sub-tetrahedra after one  $k$ -refinement (right),  $k = \frac{|x_0x_{01}|}{|x_0x_1|} = \frac{|x_0x_{02}|}{|x_0x_2|} = \frac{|x_0x_{03}|}{|x_0x_3|}$ .

**Theorem 3.1.** *There exists a sequence  $\mathcal{T}_n$  of meshes of  $\mathbb{T}$  that depends only on the choice of a parameter  $k \leq 2^{-m/a}$ ,  $0 < a < \eta$  and  $a \leq m$ , with the following property. If  $u \in \mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S})$ , then the modified Lagrange interpolant  $u_{I, \mathcal{T}_n} \in S(\mathcal{T}_n, m)$  of  $u$  satisfies*

$$\|u - u_{I, \mathcal{T}_n}\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S})},$$

where  $C$  depends only on  $m$  and  $a$  (so it is independent of  $n$  and  $u$ ).

In this section we will define the mesh refinement process and prove Theorem 3.1. The first step is to describe the refinement procedure that results in our sequence of meshes (or triangulations). This is based on the construction in [6] and in [8], thus we refer the reader to those papers for details, and here give only an outline and state the critical properties. The second step is to prove a sequence of simple lemmas used in the estimates. The third step is to prove the estimate separately on smaller regions. This uses the scaling properties of the meshes in Lemmas 2.4 and 2.5 together with Theorem 2.3.

**3.1. Construction of the meshes.** We continue to keep the approximation degree  $m$  fixed throughout this section. Fix a parameter  $a$  and let  $k = 2^{-m/a}$ . In our estimates, we will choose  $a$  such that  $a < \eta := \min_p \sqrt{1/4 + Z(p)}$  and  $a \leq m$ . Let  $l$  denote the smallest distance between the points in  $\mathcal{S}$ . Choose an initial mesh  $\mathcal{T}_0$  of  $\mathbb{P}$  with tetrahedra such that all singular points of  $V$  (i.e., all points of  $\mathcal{S}$ ) are among the vertices of  $\mathcal{T}_0$  and no tetrahedron has more than one vertex in  $\mathcal{S}$ . We assume that this mesh is such that if  $F_1$  and  $F_2$  are two opposite faces of  $\mathbb{P}$ , which hence correspond to each other through periodicity, then the resulting triangulations of  $F_1$  and  $F_2$  will also correspond to each other, that is, they are congruent in an obvious sense.

We start with a special refinement of an arbitrary tetrahedron  $T$  that has one of the vertices in the set  $\mathcal{S}$ . Our assumptions then guarantee that all the other vertices of  $T$  will not be in  $\mathcal{S}$ . Motivated by the refinement in [8, 6, 12, 13, 27], we define our  $k$ -refinement algorithm for a single tetrahedron that divides  $T$  into eight sub-tetrahedra as follows.

**Algorithm 3.2.  $k$ -refinement for a single tetrahedron:** Let  $x_0, x_1, x_2, x_3$  be the four vertices of  $T$ .

We denote  $T$  by its vertex set  $\{x_0, x_1, x_2, x_3\}$ . Suppose that  $x_0 \in \mathcal{S}$ , so that  $x_0$  is the one and only vertex that will be refined with a ratio  $k \in (0, 1/2]$ . We first generate new nodes  $x_{ij}$ ,  $0 \leq i < j \leq 3$ , on each edge of  $T$ , such that  $x_{ij} = (x_i + x_j)/2$  for  $1 \leq i < j \leq 3$  and  $x_{0j} = (1 - k)x_0 + kx_j$  for  $1 \leq j \leq 3$ . Note that the node  $x_{ij}$  is on the edge connecting  $x_i$  and  $x_j$ . Connecting these nodes  $x_{ij}$  on all the faces, we obtain 4 sub-tetrahedra and one octahedron. The octahedron then is cut into four tetrahedra using  $x_{13}$  as the common vertex. Therefore, after one refinement, we obtain eight sub-tetrahedra (Figure 1), namely,

$$\begin{aligned} &\{x_0, x_{01}, x_{02}, x_{03}\}, \{x_1, x_{01}, x_{12}, x_{13}\}, \{x_2, x_{02}, x_{12}, x_{23}\}, \{x_3, x_{03}, x_{13}, x_{23}\} \\ &\{x_{01}, x_{02}, x_{03}, x_{13}\}, \{x_{01}, x_{02}, x_{12}, x_{13}\}, \{x_{02}, x_{03}, x_{13}, x_{23}\}, \{x_{02}, x_{12}, x_{13}, x_{23}\}. \end{aligned}$$

*Algorithm 3.3.  $k$ -refinement for a mesh:* Let  $\mathcal{T}$  be a triangulation of the domain  $\mathbb{P}$  such that all points in  $\mathcal{S}$  are among the vertices of  $\mathcal{T}$  and no tetrahedron contains more than one point in  $\mathcal{S}$  among its vertices. Then we divide each tetrahedron  $T$  of  $\mathcal{T}$  that has a vertex in  $\mathcal{S}$  using the  $k$ -refinement and we divide each tetrahedron in  $T$  that has no vertices in  $\mathcal{S}$  using the  $1/2$ -refinement. The resulting mesh will be denoted  $k(\mathcal{T})$ . We then define  $\mathcal{T}_n = k^n(\mathcal{T}_0)$ , where  $\mathcal{T}_0$  is the initial mesh of  $\mathbb{P}$ .

*Remark 3.4.* According to [8], when  $k = 1/2$ , which is the case when the tetrahedron under consideration is away from  $\mathcal{S}$ , the recursive application of Algorithm 3.2 on the tetrahedron generates tetrahedra within at most three similarity classes. On the other hand, if  $k < 1/2$ , the eight sub-tetrahedra of  $T$  are not necessarily similar. Thus, with one  $k$ -refinement, the sub-tetrahedra of  $T$  may belong to at most eight similarity classes. Note that the first sub-tetrahedra in Algorithm 3.2 is similar to the original tetrahedron  $T$  with the vertex  $x_0 \in \mathcal{S}$  and therefore, a further  $k$ -refinement on this sub-tetrahedron will generate eight children tetrahedra within the same eight similarity classes as sub-tetrahedra of  $T$ . Hence, successive  $k$ -refinements of a tetrahedron  $T$  in the initial triangulation  $\mathcal{T}_0$  will generate tetrahedra within at most three similarity classes if  $T$  has no vertex in  $\mathcal{S}$ . On the other hand, successive  $k$ -refinements of a tetrahedron  $T$  in the initial triangulation will generate tetrahedra within at most  $1 + 7 \times 3 = 22$  similarity classes if  $T$  has a point in  $\mathcal{S}$  as a vertex. Thus, our  $k$ -refinement is conforming and yields only non-degenerate tetrahedra, all of which will belong to only finitely many similarity classes.

*Remark 3.5.* Recall that our initial mesh  $\mathcal{T}_0$  has matching restrictions to corresponding faces. Since the singular points in  $\mathcal{S}$  are not on the boundary of  $\mathbb{P}$ , the refinement on opposite boundary faces of  $\mathbb{P}$  is obtained by the usual mid-point decomposition. Therefore, the same matching property will be inherited by  $\mathcal{T}_n$ . In particular, we can extend  $\mathcal{T}_n$  to a mesh in the whole space by periodicity. We will, however, not make use of this periodic mesh on the whole space.

For each point  $p \in \mathcal{S}$  and each  $j$ , we denote by  $\mathcal{V}_{pj}$  the union of all tetrahedra of  $\mathcal{T}_j$  that have  $p$  as a vertex. Thus  $\mathcal{V}_{pj}$  is obtained by scaling the tetrahedra in  $\mathcal{V}_{p0}$  by a factor of  $k^j$  with center  $p$ . In particular, the level  $n \geq j$  refinements of  $\mathcal{T}_0$  give rise to a mesh on  $\mathcal{R}_{pj} := \mathcal{V}_{p(j-1)} \setminus \mathcal{V}_{pj}$ . Define

$$\Omega := \mathbb{P} \setminus \cup_{p \in \mathcal{S}} \mathcal{V}_{p0}.$$

According to Definition 3.3, both  $\Omega$  and  $\cup_{p \in \mathcal{S}} \mathcal{V}_{p0}$  are triangulated using the  $k$ -refinement. For each tetrahedron in  $\mathcal{V}_{p0}$  we use the  $k$ -refinement for a single tetrahedron, while for  $\Omega$  we use the  $1/2$ -refinement for meshes, which is, of course, a uniform refinement. Then, we can decompose  $\mathbb{P}$  as the union

$$(11) \quad \mathbb{P} = \Omega \cup_{p \in \mathcal{S}} \left( \cup_{j=1}^n \mathcal{R}_{pj} \cup \mathcal{V}_{pn} \right),$$

where each set in the union is a union of tetrahedra in  $\mathcal{T}_n$ .

*Remark 3.6.* Note that the size of each simplex of  $\mathcal{T}_n$  contained in  $\Omega$  is  $\mathcal{O}(2^{-n})$ , the size of each simplex of  $\mathcal{T}_n$  contained in  $\mathcal{R}_{pj}$  is  $\mathcal{O}(k^j 2^{-(n-j)})$ , and the size of  $\mathcal{V}_{pn}$  is  $\mathcal{O}(k^n)$ . In addition, the number of tetrahedra in  $\mathcal{T}_n$  is  $\mathcal{O}(2^{3n})$  (see Algorithm 3.3).

We now define the finite element approximation  $u_n \in S(\mathcal{T}_n, m)$  to the equation  $(L + H_{\mathbf{k}})v = f$ , where  $\mathcal{T}_n$  is obtained by applying  $n$  times the  $k$ -refinements to  $\mathcal{T}_0$ , where  $k = 2^{-m/a}$ ,  $0 < a < \eta$ ,  $a \leq m$ , and  $\lambda > 0$  satisfies Theorem 2.1. Then  $u_n$  is defined for any  $v_n \in S(\mathcal{T}_n, m)$  by

$$(12) \quad (H_{\mathbf{k}} u_n, v_n) + \lambda(u_n, v_n) := (\nabla u_n, \nabla v_n)_{L^2} + ((V + \lambda)u_n, v_n)_{L^2} = (f, v_n)_{L^2}.$$

Note that Theorem 2.1 gives that the finite element solution  $u_n \in S(\mathcal{T}_n, m) \subset \mathcal{K}_1^1$  is well defined by (12). The approximation properties of  $u_n$  are discussed in Theorem 1.1.

**3.2. Proof of Theorem 3.1.** Note that the singular expansion of Theorem 2.2 shows that the value of an eigenvalue  $u$  of  $H_{\mathbf{k}}$  at a singular point in  $\mathcal{S}$  may not be defined. Therefore, we must define the *modified* degree  $m$  Lagrange “interpolant”  $u_{I,n} = u_{I,\mathcal{T}_n}$  associated to the mesh  $\mathcal{T}_n$ , such that

$$(13) \quad \begin{cases} u_{I,n}(x) = u(x) \text{ for any node } x \notin \mathcal{S} \\ u_{I,n}(x) = 0 \text{ if } x \in \mathcal{S}. \end{cases}$$

Alternatively, we can take the modified Lagrange interpolant to be zero on the whole tetrahedron that contains a singular point. By construction, the restriction of  $\mathcal{T}_n$  to  $\mathcal{R}_{pj}$  scales to the restriction of  $\mathcal{T}_{n-j+1}$  to  $\mathcal{R}_{p1}$ . From now on, we refer to  $u_{I,n} = u_{I,\mathcal{T}_n}$  as the *modified* interpolation defined in (13). The following lemma is based on the definition of the  $k$ -refinement and the discussion in Remark 3.6.

**Lemma 3.7.** *For all  $x \in \mathcal{R}_{pj}$ ,  $u_{I,n}(x) = u_{I,n-j+1}(k^{-(j-1)}(x))$ , where  $k^{-(j-1)}(x) := p + (x - p)/k^{(j-1)}$  is the dilation with ratio  $k^{-(j-1)}$  and center  $p$ .*

Recall that  $\rho^2 V \in C^\infty(\overline{\mathbb{T} \setminus \mathcal{S}}) \cap \mathcal{C}(\mathbb{T})$  and  $\min_p Z(p) > -1/4$ . That is,  $V$  satisfies Assumptions 1 and 2.

We can now give the proof of Theorem 3.1.

*Proof.* Recall that  $\mathcal{V}_{p0}$  consists of the tetrahedra of the initial mesh  $\mathcal{T}_0$  that have  $p$  as a vertex and that all the regions  $\mathcal{V}_p$  are away from each other (they are closed and disjoint). We used this to define  $\Omega := \mathbb{P} \setminus \cup_p \mathcal{V}_{p0}$ . The region  $\mathcal{V}_{pj}$  is obtained by dilating  $\mathcal{V}_p$  with the ratio  $k^j < 1$  and center  $p$ . Finally, recall that  $\mathcal{R}_{pj} = \mathcal{V}_{p(j-1)} \setminus \mathcal{V}_{pj}$ . Let  $R$  be any of the regions  $\Omega$ ,  $\mathcal{R}_{pj}$ , or  $\mathcal{V}_{pn}$ . Since the union of these regions is  $\mathbb{P}$ , it is enough to prove that

$$\|u - u_{I,\mathcal{T}_n}\|_{\mathcal{K}_1^1(R \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|u\|_{\mathcal{K}_{a+1}^{m+1}(R \setminus \mathcal{S})},$$

for a constant  $C$  independent of  $R$  and  $n$ . The result will follow by squaring all these inequalities and adding them up. In fact, since  $\dim(S_n)^{-m/3} = \mathcal{O}(2^{-nm})$ , it is enough to prove

$$(14) \quad \|u - u_{I,\mathcal{T}_n}\|_{\mathcal{K}_1^1(R \setminus \mathcal{S})} \leq C 2^{-nm} \|u\|_{\mathcal{K}_{a+1}^{m+1}(R \setminus \mathcal{S})},$$

again for a constant  $C$  independent of  $R$  and  $n$ .

If  $R = \Omega := \mathbb{P} \setminus \cup_p \mathcal{V}_{p0}$ , the estimate in (14) follows right away from Theorem 2.3. For the other estimates, recall that  $0 < k \leq 2^{-m/a}$ , where  $0 < a < \eta$  and  $a \leq m$ . We next establish the desired interpolation estimate on the region  $R = \mathcal{R}_{pj}$ , for any fixed  $p \in \mathcal{S}$  and  $j = 1, 2, \dots, n$ . Let  $\hat{u}(x) = u(k^{j-1}x)$ . From Lemmas 2.4 and 3.7, we have

$$\|u - u_{I,n}\|_{\mathcal{K}_1^1(\mathcal{R}_{pj})} = (k^{j-1})^{1/2} \|\hat{u} - \widehat{(u_{I,n})}\|_{\mathcal{K}_1^1(\mathcal{R}_{p1})} = (k^{j-1})^{1/2} \|\hat{u} - \hat{u}_{I,n-j+1}\|_{\mathcal{K}_1^1(\mathcal{R}_{p1})}.$$

Since  $\mathcal{K}_a^m(\mathcal{R}_{p1})$  is equivalent to  $H^m(\mathcal{R}_{p1})$ , we can apply Theorem 2.3 with  $h = \mathcal{O}(2^{-(n-j+1)})$  to get

$$(15) \quad \|u - u_{I,n}\|_{\mathcal{K}_1^1(\mathcal{R}_{pj})} \leq C (k^{j-1})^{1/2} 2^{-m(n-j+1)} \|\hat{u}\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{R}_{p1})}.$$

Now applying Lemma 2.4 to scale back again and using also  $k = 2^{-m/a}$ , we get that the right hand side in (15)

$$\begin{aligned} C (k^{j-1})^{1/2} 2^{-m(n-j+1)} \|\hat{u}\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{R}_{p1})} &= C (k^{j-1})^a 2^{-m(n-j+1)} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{R}_{pj})} \\ &\leq C 2^{-mn} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{R}_{pj})}. \end{aligned}$$

This proves the estimate in (14) for  $R = \mathcal{R}_{pj}$ .

It remains to prove this estimate for  $R = \mathcal{V}_{pn}$ . For any function  $w$  on  $\mathcal{V}_{pn}$ , we let  $\hat{w}(x) = w(k^n x)$  be a function on  $\mathcal{V}_p$ . Therefore, by Lemma 2.4

$$(16) \quad \|u - u_{I,n}\|_{\mathcal{K}_1^1(\mathcal{V}_{pn})} = (k^n)^{1/2} \|\widehat{u - u_{I,n}}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}$$



and by 3.7 (which follows from the definition of the meshes  $\mathcal{T}_k$  and from the fact that interpolation commutes with changes of variables),

$$(17) \quad (k^n)^{1/2} \|u - \widehat{u_{I,n}}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} = (k^n)^{1/2} \|\hat{u} - \hat{u}_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}.$$

Now let  $\chi$  be a smooth cutoff function on  $\mathcal{V}_p$  such that  $\chi = 0$  in a neighborhood of  $p$  and  $= 1$  at every other node of  $\mathcal{V}_p$ .

Define  $\hat{v} := \hat{u} - \chi \hat{u}$ . Then, by (13),

$$(18) \quad \begin{aligned} (k^n)^{1/2} \|\hat{u} - \hat{u}_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} &= (k^n)^{1/2} \|\hat{v} + \chi \hat{u} - \hat{u}_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} \\ &\leq (k^n)^{1/2} (\|\hat{v}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi \hat{u} - \hat{u}_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}) \\ &= (k^n)^{1/2} (\|\hat{v}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi \hat{u} - (\chi \hat{u})_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}). \end{aligned}$$

Since  $\chi$  vanishes in the neighborhood of  $p$  we can consider multiplication by  $\chi$  as  $\rho^\infty$  times a degree 0 b-operator. Thus it is a bounded operator on any weighted Sobolev space. Thus

$$(19) \quad \|\hat{v}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} \leq \|\hat{v}\|_{\mathcal{K}_1^m(\mathcal{V}_p)} \leq \|\hat{u}\|_{\mathcal{K}_1^m(\mathcal{V}_p)} + \|\chi \hat{u}\|_{\mathcal{K}_1^m(\mathcal{V}_p)} \leq C \|\hat{u}\|_{\mathcal{K}_1^m(\mathcal{V}_p)},$$

where  $C$  depends on  $m$  and, through  $\chi$ , the nodes in the triangulation.

Using (16), (17), (18), (19), Lemma 2.5, and Theorem 2.3, we have

$$\begin{aligned} \|u - u_{I,n}\|_{\mathcal{K}_1^1(\mathcal{V}_{pn})} &\leq C(k^n)^{1/2} (\|\hat{u}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi \hat{u} - (\chi \hat{u})_{I,0}\|_{\mathcal{K}_1^1(\mathcal{V}_p)}) \\ &\leq C(k^n)^{1/2} (\|\hat{u}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\chi \hat{u}\|_{H^{m+1}(\mathcal{V}_p)}) \\ &\leq C(k^n)^{1/2} (\|\hat{u}\|_{\mathcal{K}_1^1(\mathcal{V}_p)} + \|\hat{u}\|_{\mathcal{K}_1^{m+1}(\mathcal{V}_p)}) \\ &\leq C \|u\|_{\mathcal{K}_1^{m+1}(\mathcal{V}_{pn})} \leq C k^{na} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{V}_{pn})} \leq C 2^{-mn} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathcal{V}_{pn})}. \end{aligned}$$

This proves the estimate of Equation (14) for  $R = V_{pn}$  and completes the proof of Theorem 3.1.  $\square$

#### 4. APPLICATIONS TO FINITE ELEMENT METHODS

We can now turn to the proofs of the theorems stated in the introduction. First, Theorem 1.1 follows from our general approximation result, Theorem 3.1, and the standard results on approximations of eigenvalues and eigenvectors (eigenfunctions in our case) discussed, for instance, in [3, 5, 4, 10, 30]. More precisely, using the notation introduced in the introduction, we have the following. Let us denote by  $E(\lambda)$  the eigenspace of  $H_{\mathbf{k}}$  corresponding to the eigenvalue  $\lambda$  and by  $E_1(\lambda) \subset E(\lambda)$ , the subspace consisting of vectors of length one. Then the following result is well known (see for instance Equations (1.1) and (1.2) in [5]). We state it only for our operator  $H_{\mathbf{k}}$ , although it is valid for more general self-adjoint operators with compact resolvent.

**Theorem 4.1.** *There exists a constant  $C > 0$  with the following property. Let  $V \subset \mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})$  be a finite dimensional subspace and  $R : \mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S}) \rightarrow V$  the projection in the energy norm. Let  $w_{j,n} \in V$  be an eigenbasis of  $RH_{\mathbf{k}}R$ , namely  $RH_{\mathbf{k}}Rw_{j,n} = RH_{\mathbf{k}}w_{j,n} = \lambda_{j,n}w_{j,n}$ , with the  $\lambda_{j,n}$  arranged in increasing order in  $j$ . Then*

$$|\lambda_j - \lambda_{j,n}| \leq C \sup_{u \in E_1(\lambda)} \inf_{\chi \in V} \|u - \chi\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})}^2$$

and, furthermore

$$\|v_j - w_{j,n}\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \sup_{u \in E_1(\lambda)} \inf_{\chi \in V} \|u - \chi\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})},$$

for a suitable eigenvector  $u_j \in E(\lambda_j)$ .

The proof of Theorem 1.1 will then be obtained from Theorem 4.1 as follows.

*Proof.* (of Theorem 1.1). We need to estimate  $\sup_{u \in E_1(\lambda)} \inf_{\chi \in S_n} \|u - \chi\|_{\mathcal{K}_1^1}$ . To this end, let us notice that any  $u \in E(\lambda) \subset \mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})$  satisfies  $(\mu + H_{\mathbf{k}})u = (\mu + \lambda)u$ . Theorem 2.1 then gives  $\|u\|_{\mathcal{K}_{a+1}^{m+1}} \leq C_{m,\lambda} \|u\|_{\mathcal{K}_{a-1}^{m-1}}$  for a suitably large  $\mu$  that depends on  $\lambda$  and  $a < \eta$ . A bootstrap argument then gives for any  $u \in E(\lambda)$  that  $\|u\|_{\mathcal{K}_{a+1}^{m+1}} \leq C'_{m,\lambda} \|u\|_{\mathcal{K}_1^1}$ . Theorem 3.1 then gives for  $u \in E_1(\lambda_j)$  (thus  $\|u\|_{\mathcal{K}_1^1} = 1$ ), the following.

$$\begin{aligned} \sup_{u \in E_1(\lambda)} \inf_{\chi \in S_n} \|u - \chi\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} &\leq \sup_{u \in E_1(\lambda)} \|u - u_{I,\mathcal{T}_n}\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \\ &\leq C \sup_{u \in E_1(\lambda)} \dim(S_n)^{-m/3} \|u\|_{\mathcal{K}_{a+1}^{m+1}(\mathbb{T} \setminus \mathcal{S})} \leq c(m, \lambda_j) \dim(S_n)^{-m/3}. \end{aligned}$$

The proof of Theorem 1.1 is now complete.  $\square$

Next, the proof of Theorem 1.2 follows from Theorem 3.1, the Lax-Milgram Lemma and Cea's lemma. We note some consequences of this theorem.

*Remark 4.2.* First, in the case  $f \in H^{m-1}(\mathbb{T} \setminus \mathcal{S})$ , by the estimate in Equation (8), we have

$$\|v - v_n\|_{\mathcal{K}_1^1(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|f\|_{\mathcal{K}_{a-1}^{m-1}(\mathbb{T} \setminus \mathcal{S})} \leq C \dim(S_n)^{-m/3} \|f\|_{H^{m-1}(\mathbb{T} \setminus \mathcal{S})},$$

as long as the index in Theorem 1.2 is chosen such that  $0 < a \leq 1$ .

As in the classical Finite Element Method, a duality argument yields the following  $L^2$ -convergence result.

**Theorem 4.3.** *In addition to the assumptions and notation in Theorem 1.2, assume that  $0 < a \leq 1$ . Then the following  $L^2$  estimate holds*

$$\|v - v_n\|_{L^2(\mathbb{T})} \leq C \dim(S_n)^{(-m-1)/3} \|f\|_{H^{m-1}(\mathbb{T})}.$$

*Proof.* We sketch the proof by using the duality argument in weighted Sobolev spaces. Consider the equation

$$(20) \quad (L + H_{\mathbf{k}})w = v - v_n \quad \text{in } \mathbb{T}.$$

(So we use periodic boundary conditions on  $\mathbb{P}$ .) The definition of the Galerkin projection  $v_n$  of  $v$ , Equation (7), then gives

$$(v - v_n, v - v_n) = ((L + H_{\mathbf{k}})w, v - v_n) = ((L + H_{\mathbf{k}})(w - w_n), v - v_n),$$

where  $w_n$  is the finite element solution of Equation (20) on  $\mathcal{T}_n$ . We also have  $\|w\|_{\mathcal{K}_{a+1}^2(\mathbb{T} \setminus \mathcal{S})} \leq C \|v - v_n\|_{L^2(\mathbb{T})}$  by Theorem 2.1, since  $v - v_n \in L^2(\mathbb{T}) \subset \mathcal{K}_{a-1}^0(\mathbb{T} \setminus \mathcal{S})$ . Therefore, applying Theorem 1.2 to  $v - v_n \in L^2(\mathbb{T})$  and  $m = 1$ , we have

$$\begin{aligned} \|v - v_n\|_{L^2(\mathbb{T})} &\leq C \|w - w_n\|_{\mathcal{K}_1^1(\mathbb{T})} \|v - v_n\|_{\mathcal{K}_1^1(\mathbb{T})} / \|v - v_n\|_{L^2(\mathbb{T})} \\ &\leq C \dim(S_n)^{-1/3} \|v - v_n\|_{\mathcal{K}_1^1(\mathbb{T})} \leq C \dim(S_n)^{(-m-1)/3} \|f\|_{H^{m-1}(\mathbb{T})}. \end{aligned}$$

This completes the proof.  $\square$

**4.1. Condition number of the stiffness matrix.** It is important that the discrete system  $S_n$  that we use is well-conditioned for us to be able to realise the theoretical approximation bounds in practice. Thus we need to additionally obtain upper and lower bounds on the eigenvalues of the stiffness matrix that arises in calculation.

Recall the standard nodal basis function  $\phi_j$  of the space  $S_n := S(\mathcal{T}_n, m)$ . It consists of functions that are equal to 1 at one node and equal to zero at all the other nodes. For convenience, we now instead consider the rescaled bases  $\varphi_j := h_j^{-1/2} \phi_j$ , where  $h_j$  is the diameter of the support patch for  $\phi_j$ . Then, we consider the scaled stiffness matrix

$$(21) \quad A_n := (a(\varphi_i, \varphi_j))$$

from our graded finite element discretization (7). In practice,  $A_n$  can be obtained from the usual stiffness matrix  $(a(\phi_i, \phi_j))$  by a diagonal preconditioning process. We point out that similar scaled matrices were considered in [7, 26] for condition numbers of other Galerkin-based methods.

For a symmetric matrix  $A$ , we shall denote by  $\lambda_{\max}(A)$  the largest eigenvalue of  $A$  and by  $\lambda_{\min}(A)$  the smallest eigenvalue of  $A$ . Thus the spectrum of  $A$  is contained in  $[\lambda_{\min}(A), \lambda_{\max}(A)]$ , but is not contained in any smaller interval. We first have the following estimates regarding properties of functions.

**Lemma 4.4.** *Let  $T_i$  be a tetrahedron in the mesh  $\mathcal{T}_n$  and let  $\text{diam}(T_i)$  denote the diameter of  $T_i$ . Then, for any  $\mu_n \in S_n$  and  $\mu \in H^1(\Omega)$ , there exists a constant  $C > 0$  independent of  $n$ ,  $\mu_n$  and  $\mu$ , such that*

$$(22) \quad \|\mu_n\|_{H^1(T_i)} \leq C \text{diam}(T_i)^{1/2} \|\mu_n\|_{L^\infty(T_i)} \leq C \|\mu_n\|_{L^6(T_i)},$$

$$(23) \quad \|\mu\|_{L^6(\Omega)} \leq C \|\mu\|_{H^1(\Omega)}.$$

Furthermore, writing  $\mu_n = \sum c_j \varphi_j$ , where  $\varphi_j := h_j^{-1/2} \phi_j$  are rescaled basis functions, then

$$(24) \quad C^{-1/2} \sum_{j \in \text{node}(T_i)} c_j^2 \leq \text{diam}(T_i) \|\mu_n\|_{L^\infty(T_i)}^2 \leq C \sum_{j \in \text{node}(T_i)} c_j^2.$$

*Proof.* We shall show (22) and (24) since (23) is a standard result in [18]. Recall that all the tetrahedra  $T_i$  belong to a finite class of shapes (or similarity classes) in our graded triangulation. Thus, the bounded constant  $C$  in (22) follows from the inverse estimates in [11, 14].

As for (24), note  $\mu_n = \sum c_i \varphi_i = \sum \bar{c}_i \phi_i$ . Based on the definition of the basis function  $\varphi_i$  and of the graded mesh,

$$(25) \quad C^{-1} \text{diam}(T_i)^{1/2} \bar{c}_i \leq c_i \leq C \text{diam}(T_i)^{1/2} \bar{c}_i.$$

On the reference tetrahedron  $\hat{T}$ , both  $\|\hat{v}\|_{L^\infty}$  and  $(\sum_{j \in \text{node}(\hat{T})} \bar{c}_j^2)^{1/2}$  are norms for the finite element function  $\hat{v}|_{\hat{T}}$ , where  $\hat{v}$  is obtained by the usual scaling process and the summation on  $\bar{c}_j$  is for all the nodes in  $\hat{T}$ . Based on equivalence of all norms for a finite dimensional space, we have

$$C \left( \sum_{j \in \text{node}(\hat{T})} \bar{c}_j^2 \right)^{1/2} \leq \|\hat{v}\|_{L^\infty(\hat{T})} \leq C \left( \sum_{j \in \text{node}(\hat{T})} \bar{c}_j^2 \right)^{1/2}.$$

This, together with (25), implies

$$C \sum_{j \in \text{node}(T_i)} c_j^2 \leq \text{diam}(T_i) \|v\|_{L^\infty(T_i)}^2 \leq C \sum_{j \in \text{node}(T_i)} c_j^2,$$

which completes the proof.  $\square$

Therefore, we have the following estimates on the eigenvalues of the stiffness matrix.

**Lemma 4.5.** *Let  $A_n$  be the stiffness matrix from the finite element discretization corresponding to the rescaled nodal basis  $\varphi_j$  of the space  $S_n := S(\mathcal{T}_n, m)$  in Equation (21). Then,*

$$\lambda_{\max}(A_n) \leq M,$$

where the constant  $M$  is independent of the mesh level  $n$ .

*Proof.* Let us fix the mesh level  $n$ . All the constants below will be independent of  $n$ . Let  $\{T_i\}$  be the tetrahedra forming our mesh  $\mathcal{T}_n$ . Let  $v \in S_n$  be arbitrary and write  $v = \sum_j c_j \varphi_j$  and  $\mathbf{V} := (c_j)$ . Then, by Lemma 3.4 in [20] we have

$$\mathbf{V}^T A_n \mathbf{V} = a(v, v) \leq C \|v\|_{\mathcal{K}_1^1(\mathbb{P})}^2 \leq C \|v\|_{H^1(\mathbb{P})}^2 \leq C \sum_i \|v\|_{H^1(T_i)}^2.$$

By the inverse inequality (22) and the estimate (24), we further have

$$\mathbf{V}^T A_n \mathbf{V} \leq C \sum_i \text{diam}(T_i) \|v\|_{L^\infty(T_i)}^2 \leq C \sum_j c_j^2 \leq C \mathbf{V}^T \mathbf{V},$$

where  $\text{diam}(T_i)$  is the diameter of the tetrahedron  $T_i$ . This completes the proof.  $\square$

**Lemma 4.6.** *We use the same notation as the one for Lemma 4.5. The smallest eigenvalue of the stiffness matrix  $A_n$ ,*

$$\lambda_{\min}(A_n) \geq C \dim(S_n)^{-2/3}.$$

*Proof.* For any  $v \in S_n$ , we use the notation  $v = \sum_j c_j \varphi_j$ ,  $\mathbf{V} := (c_j)$ , and  $\text{diam}(T_i)$  denotes the diameter of  $T_i$ , as before. In view of (24), the inverse estimate (22), Hölder's inequality, and the Sobolev embedding estimate (23), we then have

$$\begin{aligned} \mathbf{V}^T \mathbf{V} &= \sum_j c_j^2 \leq C \sum_i \text{diam}(T_i) \|v\|_{L^\infty(T_i)}^2 \leq C \sum_i \|v\|_{L^6(T_i)}^2 \\ &\leq C \left( \sum_i 1 \right)^{\frac{2}{3}} \left( \sum_i \|v\|_{L^6(T_i)}^6 \right)^{\frac{1}{3}} \leq C \dim(S_n)^{\frac{2}{3}} \|v\|_{L^6(\mathbb{P})}^2 \\ &\leq C \dim(S_n)^{\frac{2}{3}} \|v\|_{H^1(\mathbb{P})}^2 \leq C \dim(S_n)^{\frac{2}{3}} \mathbf{V}^T A \mathbf{V}. \end{aligned}$$

$\square$

Then, we have the estimate on the condition number.

**Theorem 4.7.** *Let  $A = (a(\varphi_i, \varphi_j))$  be the stiffness matrix. Then the condition number  $\kappa(A)$  satisfies*

$$\kappa(A) \leq C \dim(S_n)^{2/3}.$$

*The constant  $C$  depends on the finite element space, but not on  $\dim(S_n)$ .*

*Proof.* Using  $k(A) = \lambda_{\max}(A)/\lambda_{\min}(A)$ , we obtain the estimate by Lemmas 4.5 and 4.6.  $\square$

## 5. NUMERICAL TESTS OF THE FINITE ELEMENT METHOD

We now present the numerical tests for the finite element solution defined in (12) approximating possibly singular solutions to Equation 6.

To be more precise, suppose that our periodicity lattice is  $2\mathbb{Z}^3$  and we choose our fundamental domain  $\mathbb{P} = [-1, 1]^3$  to be a cube of side length 2. We impose periodic boundary condition on the following model problem

$$(26) \quad (L + H_{\mathbf{k}})v := (-\Delta + \delta\psi r^{-2} + L)v = 1 \quad \text{in } \Omega,$$

where  $r = |x|$ ,  $\delta > -1/4$ ,  $L \geq 0$ , and the cut-off function  $\psi := e^{r_c^2/(r^4 - r_c^2) + 1}$  for  $r^2 \leq r_c$  and  $\psi = 0$  for  $r^2 > r_c$ ; in the tests, we chose  $r_c = 0.25$ . Note that if  $\delta > 0$ , it is clear that the operator  $L + H_{\mathbf{k}}$  is positive on  $\mathcal{K}_1^1$  (see Theorem 2.1). We use the  $C^0$  linear finite element method on triangulations graded toward the origin with grading ratio  $k > 0$  (Recall that  $k = 0.5$  corresponds to the quasi-uniform refinement.)

To enforce the periodic boundary condition for the finite element functions, we use meshes where all the boundary nodal points are symmetric about the mid-plane between opposite faces of the cube. Any set of the symmetric nodes will be associated to the same shape function in the discretization. For example, nodes on edges of the cube generally have three mirror images over two mid-planes (two direct mirror images and the third is symmetric over the line of intersection of these two mid-planes), and these four points are associated to the same shape function. Consequently, the eight vertices of the cube are associated to the same shape function through symmetry. See Figure 2 for example.

Our first tests are for Equation (26) with  $\delta = 4.0$  and  $L = 0$ . According to Theorem 1.2, the optimal rate of convergence for the Finite Element solution should be obtained on triangulations with any  $k \leq 0.5$ , since  $\eta = \sqrt{1/4 + 4} > 1$ . The convergence rates  $e$  associated to triangulations with different values of  $k$  are listed in Table 1. Starting from an initial triangulation, we compute

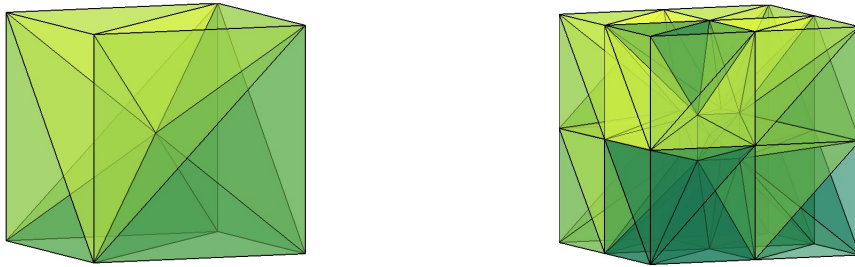


FIGURE 2. The initial mesh on the unit cube (left); the mesh after one  $k$  refinement for the origin,  $k = 0.2$  (right).

$j \backslash e$	$k = 0.1$	$k = 0.2$	$k = 0.3$	$k = 0.4$	$k = 0.5$
2	0.42	0.44	0.56	0.33	-0.20
3	0.48	0.68	0.75	0.79	0.70
4	0.78	0.81	0.86	0.88	0.85
5	0.91	0.92	0.94	0.95	0.93
6	0.97	0.97	0.98	0.99	0.98

TABLE 1. Convergence rates  $e$  of finite element solutions solving equation (26) with  $\delta = 4.0$  and  $L = 0$  on different graded tetrahedra.

the rates based on the comparison of the numerical errors on triangulations with consecutive  $k$ -refinements,

$$(27) \quad e := \log_2 \frac{|v_{j-1} - v_j|_{\mathcal{K}_1^1}}{|v_j - v_{j+1}|_{\mathcal{K}_1^1}},$$

where  $v_j$  is the finite element solution on the mesh after  $j$   $k$ -refinements. Recall the dimension of the finite element space grows by a factor of 8 with one  $k$ -refinement. By Theorem 1.2, for a sequence of optimal meshes, the error  $|v - v_j|_{\mathcal{K}_1^1}$  is reduced by a factor of 2 for linear finite element approximations with each  $k$ -refinement. Thus,  $e \rightarrow 1$  implies that the optimal rate of convergence in Theorem 1.2 is achieved.

Table 1 clearly shows that the convergence rates  $e$  approach 1 for all values of the grading parameter  $k$ . This is in agreement with our theory that the optimal rates of convergence are obtained for any triangulations with  $k \leq 0.5$ , since the singularity in the solution is not strong enough to be detectable for linear finite elements.

In the second test, we implemented our method solving equation (26) with  $\delta = 0.6$ ,  $L = 0$  and summarize the results in Table 2. Based on the upper bound  $\eta = \sqrt{1/4 + 0.6}$  given in Theorem 1.2, we expect the optimal rate of convergence for the numerical solution as long as the grading parameter  $k < 2^{-1/\eta} \approx 0.47$ . The convergence rates in Table 2 tend to 1 when  $k \leq 0.4$ , which implies the optimality of our finite element approximation on these meshes. However, when  $k = 0.5$ , the convergence rate is far less than 1 and there is a large gap between the rates corresponding to  $k = 0.4$  and  $k = 0.5$ . This further confirms our theory that the upper bound of the suitable range of  $k$  for an optimal finite element approximation lies in  $(0.4, 0.5)$ .

The third tests are for negative potentials in equation (26), where we set  $\delta = -0.1$  and  $L = 20$  to satisfy the positivity requirement in Theorem 2.1. Our theoretical results indicate that the singularity in the solution due to the singular potential is stronger in this case and the optimal rate can be achieved only if the grading parameter  $k < 2^{-1/\sqrt{1/4-0.1}} \approx 0.167$ . Because of the limitation of the computation power, we only display the convergence results up to the 7th refinement for various graded parameters  $k$  in Table 3. We, however, still see the trend that appropriate gradings improve the convergence rate as predicted in Theorem 1.2. When  $k$  is close

$j \backslash e$	$k = 0.1$	$k = 0.2$	$k = 0.3$	$k = 0.4$	$k = 0.5$
2	0.20	0.30	0.33	0.11	-0.03
3	0.54	0.66	0.69	0.61	0.39
4	0.74	0.81	0.83	0.77	0.60
5	0.88	0.91	0.92	0.87	0.72
6	0.95	0.97	0.98	0.92	0.79

TABLE 2. Convergence rates  $e$  of finite element solutions solving equation (26) with  $\delta = 0.6$  and  $L = 0$  on different graded tetrahedra.

$j \backslash e$	$k = 0.1$	$k = 0.2$	$k = 0.3$	$k = 0.4$	$k = 0.5$
2	-0.10	-0.05	-0.09	-0.16	-0.03
3	0.32	0.37	0.30	0.19	0.07
4	0.51	0.52	0.44	0.32	0.18
5	0.67	0.64	0.53	0.40	0.26
6	0.80	0.72	0.59	0.45	0.32

TABLE 3. Convergence rates  $e$  of finite element solutions solving equation (26) with  $\delta = -0.1$  and  $L = 20$  on different graded tetrahedra.

to the optimal value 0.167 (i.e.,  $k = 0.1$  and  $0.2$ ), we have remarkable improvements. In particular, for  $k = 0.1$ , based on Table 3, we expect that the optimal rate occurs with further refinements.

We have also implemented the method on graded meshes for the eigenvalue problem associated with equation (26), especially on the computation of the first eigenvalues. Namely,

$$H_{\mathbf{k}}u := (-\Delta + \delta\psi r^{-2})u = \lambda_1 u$$

on the unit cube, where  $\lambda_1$  is the first eigenvalue of the operator. Depending on the choice of  $\delta$ , the convergence rates for the numerical eigenvalues on graded meshes are roughly twice the rates for the numerical solutions of equation (26) (see Tables 1, 2, and 3), and present similar trends for different gradings.

All our numerical tests (Tables 1, 2, 3, and corresponding eigenvalue computations) convincingly verify Theorem 1.1 by comparing the rates of convergence for different singular potentials on different graded triangulations for the model operator in (26). The theoretical upper bounds  $2^{-1/\eta}$  of the optimal range for the grading parameter  $k$  are also clearly demonstrated in these numerical results. In these tests, the initial triangulation of the unit cube consists of 12 tetrahedra and we consecutively refine the mesh using the  $k$ -refinements up to level 7 that includes  $12 \times 8^7 \approx 2.5 \times 10^7$  tetrahedra and roughly 4.2 million unknowns. Numerical experiments show that the condition numbers of our discrete systems grow by a factor of 4 for consecutive refinements, regardless of the value of  $k$ , which resembles the estimates given in [7] for the Laplace operator. However, the values of  $k$  affect the magnitude of the condition numbers. In general, smaller  $k$  leads to bad shapes for the tetrahedra and therefore results in larger condition numbers. The preconditioned conjugate gradient (PCG) method was used as the numerical solver for the discrete systems.

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